

Chloroform

67-66-3 | DTXSID1020306

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.96

Global applicability domain: Outside

Local applicability domain index: 3.95e-01

Confidence level: 7.79e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Chloroform</div> <div>Measured: 1.97</div> <div>Predicted: 1.96</div>	<div>Image not found</div> <div>Trichlorofluoromethane</div> <div>Measured: 2.53</div> <div>Predicted: 2.44</div>	<div>Image not found</div> <div>3H-1,2-Dithiole-3-thione, 5-methyl-</div> <div>Measured: 1.89</div> <div>Predicted: 1.91</div>
<div>Image not found</div> <div>Bromodichloromethane</div> <div>Measured: 2.00</div> <div>Predicted: 2.04</div>		